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Strain relaxation in InAs/GaSb heterostructures

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Lattice strain relaxation in InAs/GaSb heterostructures was investigated by x-ray diffraction. Two types of structures, grown by molecular beam epitaxy, are compared. In the first, GaSb buffer layers were grown on GaAs substrates, followed by 0.05–1.0 μm thick InAs layers. In the second, InAs layers were grown directly on GaSb substrates. For a given thickness, the InAs layers retain significantly more strain when grown on GaSb substrates, reflecting the lower threading dislocation density in the GaSb substrates relative to the GaSb buffer layers grown on GaAs. [S0003-6951(98)02251-7]

Heterostructures containing InAs and GaSb are of interest for a variety of optical and electronic devices as well as fundamental studies of band structure.¹ For example, superlattices consisting of thin alternating layers of InAs and GaSb may be suitable for long-wavelength infrared detectors.² In addition, resonant tunneling diodes based upon InAs/GaSb/AlSb heterostructures have been demonstrated.³

The classic “lattice-matched” semiconductor system is GaAs/AlAs with a lattice mismatch of only 0.14%. The influence of strain on epitaxial growth of GaAs/AlGaAs heterostructures is negligible. At the other extreme are systems with large mismatches such as Si/Ge (3.9%), GaAs/Si (4.0%), InAs/GaAs (6.9%), and GaSb/GaAs (7.5%). Three-dimensional growth occurs for thin layers, with the formation of high densities of dislocations during the coalescence of islands. The InAs/GaSb system, with a 0.61% mismatch ($a_{\text{InAs}} = 6.0584 \text{ \AA}$, $a_{\text{GaSb}} = 6.0954 \text{ \AA}$), falls in an intermediate regime. The strain is too small to induce three-dimensional growth under normal conditions, but misfit dislocations will form to relieve strain if the layer thickness is too large. The classic Matthews–Blakeslee critical layer thickness (MB-CLT) for single layers of InAs on GaSb is about 200 \AA .^{4,5} Strained epilayers do not completely relax when the MB-CLT is reached. In fact, in many material systems, epilayers exceeding the MB-CLT by as much as an order of magnitude exhibit little or no lattice relaxation. This effect has been quantitatively investigated⁶ and attributed to the difficulty of generating misfit dislocations.^{5,7}

Little work related to strain relaxation in InAs/GaSb has been reported. Yang *et al.* measured strain-induced shifts in phonon energy and found that InAs films were coherently strained to GaSb for thicknesses of 60–190 \AA .⁸ Bolognesi *et al.* examined the related InAs/AlSb system (mismatch = 1.3%) and found a CLT of 220 \AA based upon low-temperature mobility measurements of single quantum well structures.⁹ In this letter, we examine a variety of InAs layers grown on GaSb. We show that the quality of the GaSb layer influences the strain relaxation in the InAs.

Samples were grown by solid-source molecular beam epitaxy (MBE). Two types of heterostructures were investigated and are illustrated in Fig. 1. In type-I structures, the

substrate is semi-insulating GaAs(001).¹⁰ A buffer layer of approximately 0.5 μm GaAs is grown at 580 $^{\circ}\text{C}$, followed by a buffer layer of GaSb at 500 $^{\circ}\text{C}$, and InAs at 450 $^{\circ}\text{C}$. The type-II structure begins with an unintentionally doped GaSb(001) substrate.¹¹ A buffer layer of approximately 0.5 μm GaSb is grown at 500 $^{\circ}\text{C}$, followed by InAs at 450 $^{\circ}\text{C}$. Growth rates were 3 $\text{\AA}/\text{s}$ and V:III flux ratios were approximately 1.5:1. Samples were characterized by double-crystal x-ray diffraction measurements (DCXRD) with a GaAs(001) first crystal oriented for the (004) reflection.

In Fig. 2, we show the DCXRD data with the (004) reflection for two samples: a type-I structure with a 4.0 μm GaSb buffer layer and a type-II structure. The InAs thickness is 1000 \AA for each. Dynamical simulations show that for fully coherent and fully relaxed epilayers of InAs on GaSb, the peak separations are 1550 and 740 arcsec, respectively. Peak separations for samples I and II are 1400 and 1480 arcsec, respectively. From the measured peak separations, we calculate the in-plane strain in the InAs and obtain 0.47% for sample I and 0.55% for sample II. In terms of epilayer quality (as measured by the peak width) and epilayer strain, sample II is superior to I.

We investigated the strain relaxation of type-II structures by varying the InAs thickness from 500 \AA to 1.0 μm . The (004) DCXRD measurements for six samples are shown in Fig. 3. The classic behavior for mismatched epilayers is for the thinnest layers to be fully strained (coherent) up to a critical thickness, with increasing lattice relaxation (decreasing $\Delta\theta$) for increasing thickness beyond the critical value. To first order, that is what we observe in Fig. 3.¹² Substantial lattice relaxation does not occur until the layer thickness reaches 3000 \AA , more than an order of magnitude larger than the Matthews–Blakeslee limit. As a result of limited resolution, DCXRD measurements are not sensitive to the onset of

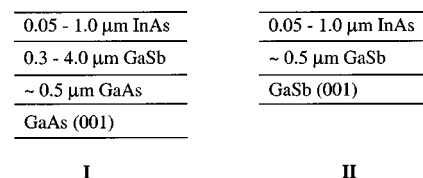


FIG. 1. Schematic of the type-I and type-II heterostructures used in this study.

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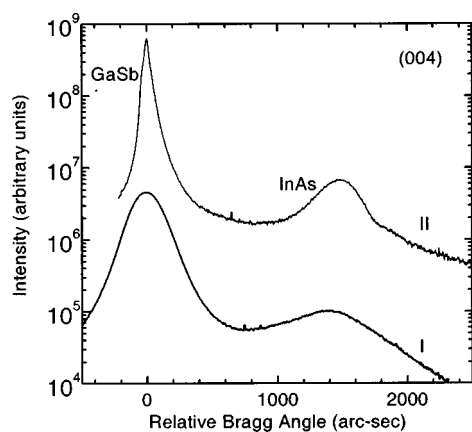


FIG. 2. Double-crystal x-ray diffraction data for two samples with 1000 Å InAs layers: (I) type-I structure with 4.0 μm GaSb buffer, (II) type-II structure.

dislocation formation.¹³ Hence, our results do not necessarily imply the absence of misfit dislocations for thinner layers. These results are relevant to the design of heterostructures in which the electronic or optical properties are sensitive to strain in the InAs.

Information about the epilayer quality can also be extracted from the data. The full width at half maximum (FWHM) is often cited as a measure of structural quality. Even for perfect layers, however, the FWHM is a function of thickness, with thinner layers having larger FWHMs because of the smaller correlation lengths. Hence, we use the ratio of the experimental to the theoretical FWHM as a figure of merit.^{14,15} For samples I and II of Fig. 2, the FWHM ratios are 3.9 and 2.0, respectively. The ratios for the samples in Fig. 3 are: 1.1 (500 Å), 2.0 (1000 Å), 2.2 (2000 Å), 16 (3000 Å), 25 (5000 Å), and 41 (10 000 Å). In addition, we observe Pendellosung fringes for the 500 Å sample, indicating good structural quality. The FWHM of the GaSb peak increases with increasing InAs thickness. Similar effects have been observed in other material systems and attributed to strain-induced lattice curvature.¹⁶

As indicated in Fig. 2, the relaxation behavior of InAs is a function of the underlying GaSb. To summarize the data from Figs. 2 and 3 as well as several additional type-I samples, we plot the epilayer strain as a function of InAs thickness in Fig. 4. In general, layers on GaAs substrates are

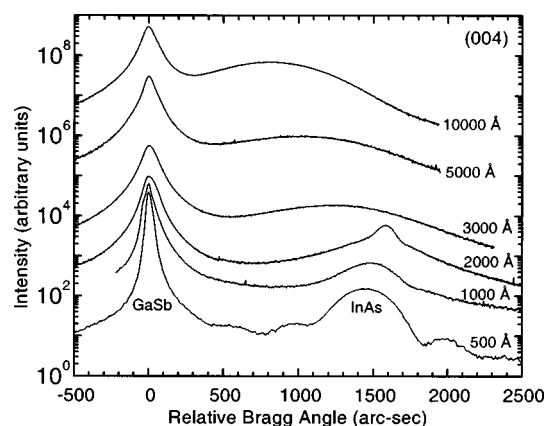


FIG. 3. Double-crystal x-ray diffraction data for six type-II structures with the indicated InAs layer thicknesses.

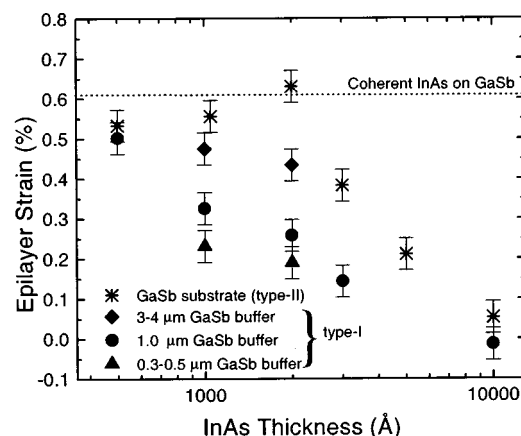


FIG. 4. InAs epilayer strain vs thickness for type-I and type-II structures.

less strained than those on GaSb substrates. For example, at a thickness of 2000 Å, InAs on a GaSb substrate is fully strained, but the strain drops to 0.2%–0.4% for GaSb buffer layers on GaAs substrates. For type-I structures, more strain is retained in the InAs layer when the GaSb buffer layer is thicker. These results are consistent with threading dislocations serving as nucleation sites for misfit dislocations. In the case of GaSb buffer layers on GaAs, high densities of threading dislocations form during the coalescence of islands.^{17–19} The dislocation density decreases as layer thickness increases. Hence, fewer nucleation sites will be available for thicker buffer layers, resulting in less relaxation of the InAs. The lowest density of threading dislocations is expected for the GaSb substrates, with etch pit densities less than $10^4/\text{cm}^2$. We note that in the InGaAs/GaAs system, the density of misfit dislocations in strained InGaAs was found to be a function of the density of threading dislocations in the GaAs substrate.^{20–22} An additional effect might account for part of the observed variation in InAs strain with buffer layer thickness. The GaSb buffer layer could act as a compliant substrate,²³ with the InAs inducing partial strain relaxation in the GaSb. Our x-ray measurements (not shown) suggest that this effect may be present but is not large enough to account for most of the observed variation in InAs strain.

Finally, we have observed that little or no improvement in InAs coherence can be achieved in type-I samples by varying such factors as doping or growth temperature, or the addition of other intermediate layers. For instance, two samples with 1.0 μm GaSb buffer layers were grown; the InAs thickness was 1000 Å for both, but the InAs growth temperature was 370 °C for one and 500 °C for the other. Within experimental error the measured strains in these two samples and the equivalent sample grown at 450 °C were equal. Previous work indicated that AlSb forms a smooth surface on GaAs faster than GaSb on GaAs.^{24,25} Following this observation, we grew a 1000 Å AlSb buffer on GaAs, followed by 1 μm GaSb and 1000 Å InAs at 450 °C. The resulting InAs strain was comparable to the equivalent sample grown without the AlSb. Addition of a short-period superlattice, $10 \times (24 \text{ Å GaSb}/24 \text{ Å AlSb})$, in the center of the GaSb buffer produced a sample which had comparable strain to an equivalent sample (2000 Å InAs) grown without the superlattice. Finally, high doping levels (Si, $n \sim 10^{19}/\text{cm}^3$) in a 2000 Å InAs sample did not appear to

affect the strain in the InAs. These results do not rule out the possibility that lattice relaxation in type-II structures could be a function of growth temperature or doping.

In summary, we applied x-ray diffraction to investigate lattice strain relaxation in MBE-grown InAs/GaSb heterostructures. We found that the strain in an InAs epilayer can be a strong function of the quality of the underlying GaSb layer. For GaSb substrates, InAs layers as thick as 2000 Å remain coherently strained, despite the 0.6% lattice mismatch.

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- ¹⁰GaAs wafers from AXT, Inc., Fremont, CA.
- ¹¹GaSb wafers from Wafer Technology Ltd., Milton Keynes, England.

- ¹²Although the value of $\Delta\theta$ for the 2000 Å layer (1580 arcsec) is very close to the theoretical value for a coherent layer (1550 arcsec using $a_{\text{InAs}} = 6.0584$ Å, $a_{\text{GaSb}} = 6.0954$ Å, $\nu_{\text{InAs}} = 0.352$, and $\nu_{\text{GaSb}} = 0.313$), the values for 500 and 1000 Å layers, 1450 and 1480 arcsec, respectively, are somewhat smaller. This discrepancy appears to be beyond the experimental uncertainty and was reproduced with single-crystal x-ray measurements. The shift is qualitatively similar to, but substantially larger than, the Fewster-Curling thin-film effect [P. F. Fewster and C. J. Curling, *J. Appl. Phys.* **62**, 4154 (1987)]. Other possibilities, including slightly off-orientation substrates and errors in Poisson's ratio, have been considered but apparently are not large enough to account for the discrepancy.
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